merlin v4: an updated platform for reconstructing genome-scale metabolic models

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The Metabolic Models Reconstruction Using Genome-Scale Information (*merlin*) software (1) is an open source user-friendly Java (2) application developed for Windows and Unix, aimed towards the reconstruction of genome-scale metabolic models. The development of merlin follows a design philosophy of automating time-consuming steps in the reconstruction of genome-scale metabolic models, while allowing users to control the parameters of operations and manually curate the results. All major steps involved in the reconstruction of a metabolic model are implemented in merlin, including genome retrieval and its functional annotation, construction of the reactions' set and associated entities, model compartmentalization and conversion to standard SBML formats (3).

The fourth iteration of *merlin* includes a major overhaul of the user interface, implementation of new features, improvements to existing features, and most notably, the implementation of the object-relational mapping framework *Hibernate* (4). The graphical layout has been significantly streamlined, while supporting the latest version of *AiBench* (5), providing users with an intuitive and responsive interface. Development was also focused at new quality of life improvements, aimed mainly towards importing, exporting and duplicating *merlin* user projects. The development of the latest version of *merlin* followed a modular approach, culminating in the implementation of a plugin manager which simplifies and hastens the process of updating and debugging the various features of *merlin*.

In addition, TranSyT, a state-of-the-art genome-wide transmembrane transport system annotation tool has been implemented to overcome the limitations of the previously available TRIAGE module (6). Finally, it is noteworthy to mention the implementation of BioISO, a tool aimed at evaluating a genome-scale metabolic network or biomass formulation, based on the previously available COBRA (7) and FBA (8) frameworks.